

Tenth DOE ACTS Collection Workshop

Leveraging the Development of Computational Science and Engineering Software Through Sustainable High Performance Tools

SUMMARY



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ACTS Collection Workshop 2009
Berkeley, California,
August 2009



A Few Summary Comments

- ♦ Tutorial materials
- ♦ What's Next
- ♦ ACTS Tools reviewed this week
- ♦ Computational Tools, Libraries and Interfaces
- ♦ Related Projects
- ♦ NERSC Accounts
- ♦ Research Opportunities

Tutorial Materials

<http://acts.nersc.gov/events/Workshop2009/>

- ◆ Tutorials and Talks
- ◆ Extra materials
 - ◆ Tutorials on related tools
 - ◆ Pointers to related project
 - ◆ References: books and articles

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What Is Next?

- ♦ What's Next

- ♦ Survey

- ♦ Periodic News

- ♦ ACTS Fellow

- New algorithmic developments
 - New tools
 - Programming/Paradigms
 - Uniform documentation/distribution/installation
(Live DVDs)

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Tuesday	Wednesday	Thursday	Friday
<i>Registration Opens</i> 7:45 AM	<i>Doors Open</i> 8:00 AM	<i>Doors Open</i> 8:00 AM	<i>Doors Open</i> 8:00 AM
<i>Welcome Remarks and Introduction</i> T. Drummond 08:30 - 09:30	<i>PETSc</i> S. Balay 08:30 - 10:30	<i>SuperLU</i> S. Li 08:30 - 09:30	<i>Vislt</i> H. Childs 08:30 - 10:30
<i>ScaLAPACK</i> T. Drummond 09:30 - 10:30		<i>Invited Talk</i> H. Simon CRD Div. Director 09:30 - 10:30	
Break 10:30 - 11:00	Break 10:30 - 11:00	Break 10:30 - 11:00	Break 10:30 - 11:00
<i>Hypre</i> R. Falgout 11:00 - 12:00	<i>SLEPc</i> J. Roman 11:00 - 12:00	<i>TAU</i> S. Shende 11:00 - 12:30	<i>CCA</i> CCA Team* 11:00 - 12:30
<i>Group Photo</i> 12:00 - 12:30	<i>CITRIS Tour</i> M. Nikraves 12:00 - 12:30		
Lunch 12:30 - 13:30	Lunch 12:30 - 13:30	Lunch 12:30 - 13:30	Lunch 12:30 - 13:30

Tuesday	Wednesday	Thursday	Friday
<i>Zoltan</i> C. Chevalier 13:30 – 14:30	<i>TAO</i> J. Sarich 13:30 – 14:30	<i>Trilinos</i> J. Hu 13:30 – 14:30	CCA Hands-On CCA TEAM* 13:30 – 16:30
<i>Global Arrays</i> B. Palmer 14:30 – 15:30	<i>Parallel I/O</i> K. Antipas 14:30 – 15:30	<i>Overture</i> B. Henshaw 14:30 – 15:30	
<i>Break</i> 15:30 – 16:00	<i>Break</i> 15:30 – 16:00	<i>Break</i> 15:30 – 16:00	
<i>ScaLAPACK</i> Hands-On T. Drummond 16:00 – 17:00	<i>PETSc</i> Hands-On S. Balay 16:00 – 17:00	<i>TAU</i> Hands-On S. Shende 16:00 – 17:00	Workshop Ends
<i>Global Arrays</i> Hands-On M. Krishnan B. Palmer 17:00 – 18:00	<i>SLEPc</i> Hands-On J. Roman 17:00 – 18:00	<i>Trilinos</i> Hands-On J. Hu 17:00 – 18:00	• CCA TEAM: David Benhadi Tamara Danilgen Wael Elwasif Tom Epperly Sameer Shende
	<i>TAO</i> Hands-On S. Sarich 18:00 – 19:00	<i>Overture</i> Hands-On B. Henshaw 18:00 – 19:00	
<i>Welcome Dinner</i> M. Nikravesh 19:00 – 21:00			

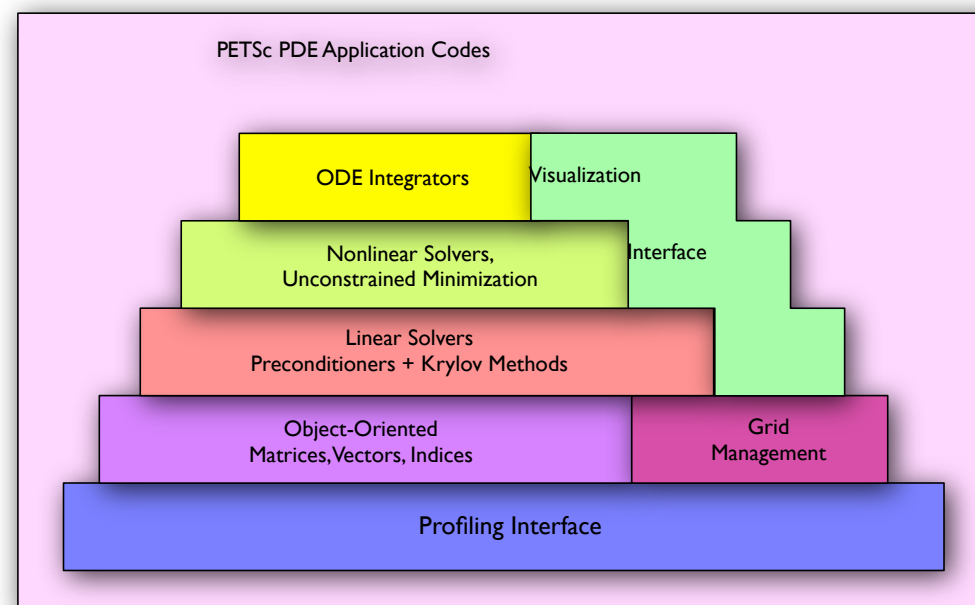
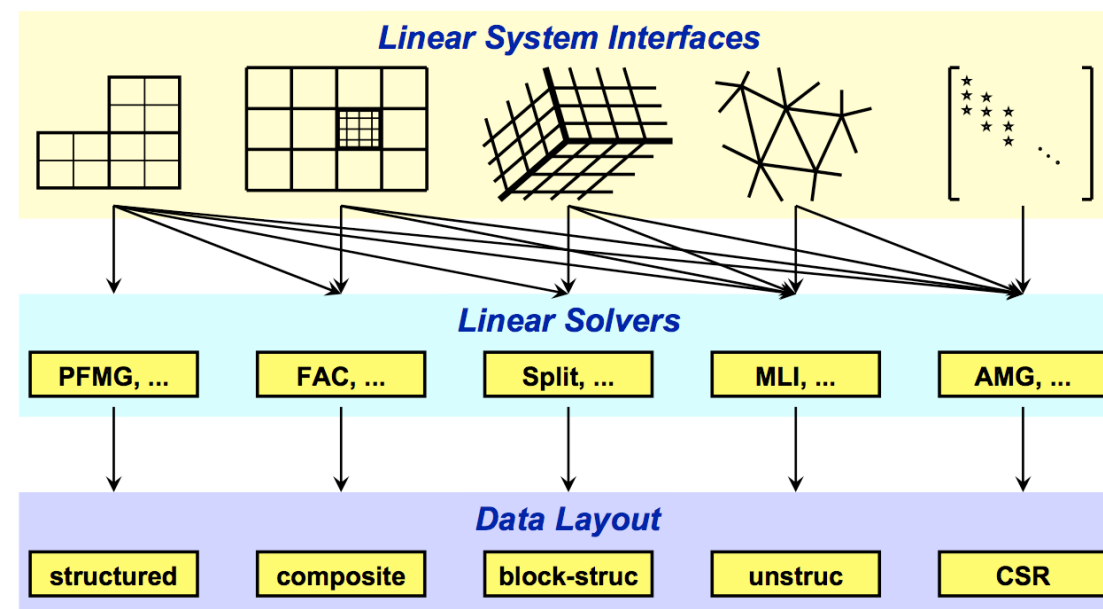
What we didn't see

- ♦ Numerical Tools
 - ♦ OPT++
 - ♦ SUNDIALS (slides available on-line)
- ♦ Library Development
 - ♦ ATLAS
- ♦ Code Execution
 - ♦ CUMULVS

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Iterative Solvers



Minimum Requirements for Sustainable Software

```
CALL BLACS_GET( -1, 0, ICTXT )
CALL BLACS_GRIDINIT( ICTXT, 'Row-major', NPROW, NPCOL )
:
CALL BLACS_GRIDINFO( ICTXT, NPROW, NPCOL, MYROW, MYCOL )
:
:
CALL PDGESV( N, NRHS, A, IA, JA, DESCA, IPIV, B, IB, JB, DESCB,
$           INFO )
```

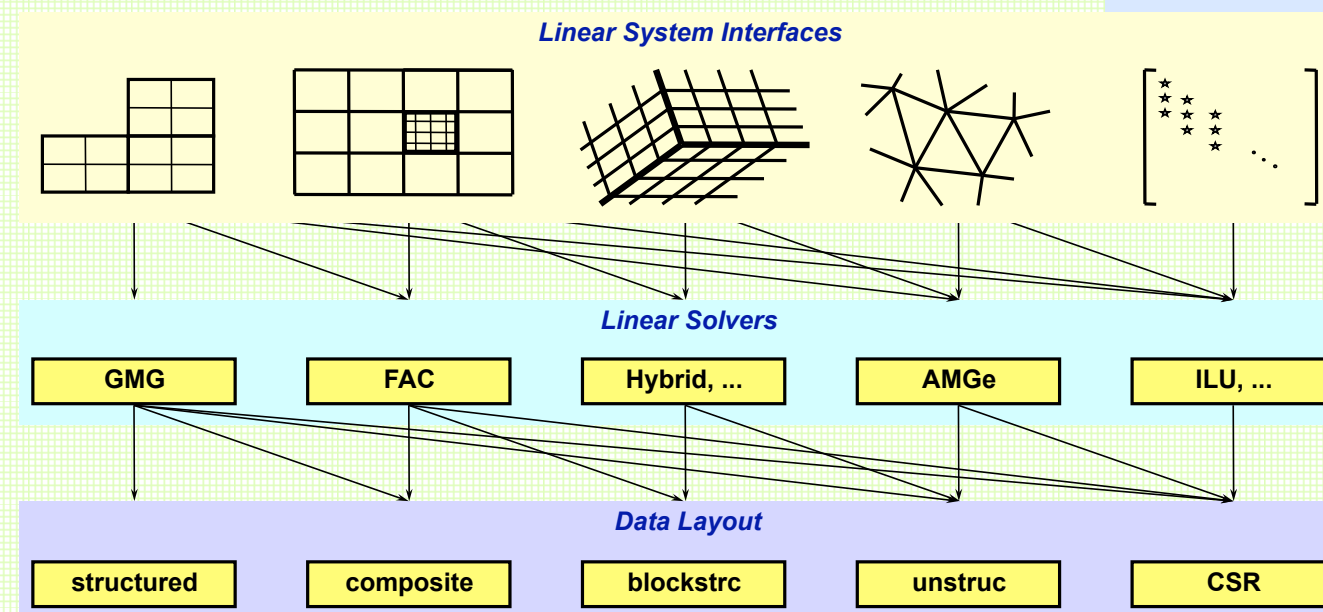
Library Calls

- `-ksp_type` [cg,gmres,bcgs,tfqmr,...]
- `-pc_type` [lu,ilu,jacobi,sor,asm,...]

More advanced:

- `-ksp_max_it` <max_iters>
- `-ksp_gmres_restart` <restart>
- `-pc_asm_overlap` <overlap>

Command lines



Problem Domain

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Related Projects

SciDAC: Scientific Discovery Through Advance Computing

- ◆ <http://www.scidac.gov/>
- ◆ Projects
 - ◆ ITAPS
 - ◆ APDEC
 - ◆ TOPS
 - ◆ TASCs

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Related Projects

- ♦ train accounts (`train1` – `train50`)
- ♦ Start-up Accounts
 - ♦ Go to NERSC.GOV
 - ♦ No cost
- ♦ Long-term: Apply

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Research Opportunities

- ◆ Send E-mail to Developers
- ◆ TAU Project
- ◆ CITRIS
- ◆ JOBS.LBNL.GOV
- ◆